AN IMPLICIT SOLVING ALGORITHM ADAPTED TO NUMERICAL IDENTIFICATION FOR SIMPLE LATTICE DISCRETE ELEMENT MODELS OF QUASI-BRITTLE MATERIALS

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Abstract. A lattice discrete element model is presented to model quasi-brittle materials behavior. The model is developed to enhance latter numerical identification and characterization of quasi-brittle materials under cyclic or multi-directional loadings. Emphasis is put on the simplicity of the description of mechanisms furthering statistical and geometrical details instead of elaborate constitutive laws; and on the accuracy and the robustness of an original implicit solving procedure.

1 Introduction

Predictive simulations of civil engineering structures require light models due to their important dimensions. In order to reduce the number of degrees of freedom in the mesh, material's models are asked to depict the behavior of at least a representative elementary volume of matter. Consequently, those macroscopic models are complex in terms of constitutive laws and parameters; and numerous experiments are then required to characterize and identify them.
However in the case of quasi-brittle material, experiments can often be difficult or even impossible to realize, because important cracking is involved. Therefore lacks of knowledge exist about the behavior quasi-brittle materials when cyclic or multi-dimensional

loadings are considered. The development of macroscopic models is still limited by these shortcomings, and influence can be felt on robustness as well as accuracy of such models.

As part of multi-scale approach, lower-scale models can be exploited to replace most of the experiments needed to identify and characterize macroscopic models [1]. Regarding quasi-brittle materials, the choice of the lower-scale model turns to lattice discrete element models [2]. Such models are adapted to account explicitly for most of the controlling phenomenons in the behavior of quasi-brittle materials, namely ones related to cracking. To be suitable for numerical experimentation, lattice discrete element models have to remain simple to depict most of loading situations with limited identification costs. In that sense, developing a simple model with physically meaningful parameters is believed to be important. Thus constitutive laws [3] such as ones used in macroscopic models are preferred to be avoided. Instead geometrical [4] and statistical [5, 6] details are preferred. Nevertheless enhancing physical sense and simplicity of the model, implies unregularized behaviors, efforts have to be made on the solving procedure to determine accurately the response of the model. Objective is to reduce bias introduced by numerical solving. Classically for discrete elements models, equilibirum is solved explicitly, due to the dynamic framework, causing dependency of the results and their precision to the time-discretization.

In order to circumvent this issue, we propose here to try an original implicit solving procedure developed for lattice discrete elements models. The paper will be outlined as follows, first the simple lattice discrete element model will be briefly presented, then the implicit solving procedure, and finally validating examples, highlighting the interest and the necessity of such approach for numerical identification purposes.

2 The lattice discrete elements model

The following section presents a lattice discrete element model based on simple force models, criterions and geometrical specificities, with an effort made on reducing the number of parameters or at least physically meaningless ones.

2.1 Cohesion

Cohesion forces are introduced between particles by means of Euler-Bernoulli beams. As a result, cohesion forces are linear elastic. Only two parameters are introduced, the Young modulus E, and a thickness ratio α. The second one is only used to compute the moment of inertia I and the cross-section area A, because the model is bi-dimensional. Its single purpose is to adjust the Poisson's ratio of the model. Otherwise, in a three-dimensional model, the moment of inertia and the cross-section would only depend on particles meshing, similarly to other beam's properties: the beam width h, the initial

length l_c.

$$\underline{F}_{coh,ij} = \begin{cases} F_{N,ij} = \dfrac{EA_{ij}}{l_{c,ij}} \left(u_i - u_j\right) \\ \\ F_{T,ij} = \dfrac{12EI_{ij}}{l_{c,ij}^3} \left(v_i - v_j\right) - \dfrac{6EI_{ij}}{l_{c,ij}^2} \left(\theta_i - \theta_j\right) \\ \\ M_{Z,ij} = \dfrac{6EI_{ij}}{l_{c,ij}^2} \left(v_j - v_i\right) + \dfrac{4EI_{ij}}{l_{c,ij}} \left(\theta_i - \dfrac{\theta_j}{2}\right) \end{cases} \tag{1}$$

where i and j are two connected particles, u, v and θ their degrees of freedom, respectively the normal displacement, the tangential displacement and the rotation.

2.2 Contact

Contact forces develop when two particles overlap. Once again, the force model used is based on beam's theory. Besides of course that contact forces are unilateral, a slight difference with the expression of cohesion forces exists. The normal strain of the beam is not expressed as the relative normal displacement of the particles centroids, but as the ratio of the overlap area S_r and the width of the overlap area. This ratio can be seen as an average indentation accounting for irregular particles shape.

$$F_{cont,ij} = -\frac{ES_{r,ij}}{l_{c,ij}} \tag{2}$$

where l_c is still a characteristic length, but since initial length has no meaning in the case of contact, l_c is defined as the actual distance between the two particles centroids.

2.3 Frictional sliding

Mechanisms relative to hysteresis effects would require introducing geometrical details from a much smaller scale, so friction is taken into account. A Coulomb's type of friction is considered introducing a single parameter, the friction coefficient μ. The elastic part, before reaching the perfectly plastic behavior of the friction force, is computed as the tangential force in beam's theory, except that the displacement used are the displacements accumulated since contact has begun u_c instead of total displacements:

$$\underline{u}_{c,ij}^{t+1} = \begin{cases} \underline{u}_{c,ij}^{t} + \underline{\delta u}_{i}^{t} & \text{if } i \text{ and } j \text{ are overlapping} \\ \\ 0 & \text{if } i \text{ and } j \text{ are distant} \end{cases} \tag{3}$$

A new internal variable δu_s measuring the sliding relative displacement between two particle is introduced and updated in order to verify Coulomb's criterion.

$$F_{fric,ij} = \min\left(\frac{EI_{ij}}{\left(l_{c,ij}\right)^3}\left[\left(\underline{u}_{c,ij} - \underline{u}_{c,ji}\right) - \underline{\delta u}_{s,ij}\right], \mu F_{N,ij}\right) \tag{4}$$

2.4 Fracture

The global failure of the material is depicted by breaking cohesive beams, when a certain combination of solicitations is locally exceeded. The criterion is chosen as a combination of strains and rotations, since extensions and bending are the main failure modes of a beam. One elastic limit is defined for each mode, in strains ϵ_{cr} and in rotations θ_{cr}. The beams are perfectly brittle, meaning that once the criterion is outreached, they are merely removed from the model not even going through a softening phase.

$$P_{ij} = \left(\frac{\epsilon_{ij}}{\epsilon_{cr,ij}}\right)^2 + \left(\frac{|\theta_i - \theta_j|}{\theta_{cr,ij}}\right) > 1 \tag{5}$$

The elastic limits are ϵ_{cr} and θ_{cr} statistically defined. Particular values for each cohesive beam are drawn from Weibull distributions assigned to ϵ_{cr} and θ_{cr}. This choice of description introduces 2 parameters for each distribution, to describe the whole fracture process. The statistical approach replicates the spatial variation of strength of the material from the mesoscopical point of view due to heterogeneities such as pores, but also the presence of uncertainties in the behavior and defects in the matter at lower scales.
Even though the fracture behavior is locally perfectly brittle, the addition of probabilistic distributions of the elastic limits allows to account for a macroscopically more ductile behavior, provided an appropriate identification.

2.5 Geometrical specificities

Meshing of a sample of matter is pursued with a Voronoi tessellation, which produces an assembly of convex polygons avoiding creation of undesired porosity. Particles centroids are randomly distributed in a grid overlaying the sample, which size controls particles density. This leads to an irregularly shaped particles with relatively similar areas. The cohesive beams are placed between centroids, and their width depends on length of the common side of the connected particles. Thus cohesive beams have random orientations as well as random stiffness. This ensures isotropy of whole model's behavior, elastically as well as inelastically. The random distribution of the elastic properties with no correlation to the probabilistic distribution of fracture thresholds amplifies the consideration of uncertainties and defects. Incidentally, size-effects is well described.

3 Implicit solving procedure

Classically in implicit integration schemes, equilibrium equations are solved iteratively until they are verified with all variables being expressed at the current time. This process usually requires to recursively predict and correct the values of the variables of the problem. It is exactly the methodology that we are going to apply to address all the non-linearities of the problem, except cracking.
In lattice discrete elements models cracking is computed by removing beams when the

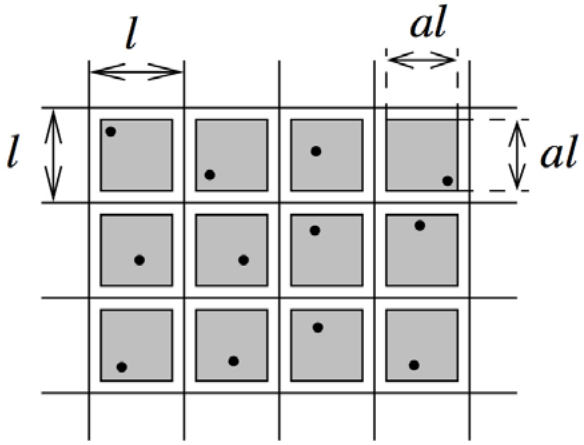


Figure 1: Random disposition of centroid nodes in an actual area of size al^2 [1]

criterion aforementioned is exceeded. An explicit method would simply remove every broken beam of the system at the end of the time-step and go on to the next one. Actually, not much work is needed to solve cracking implicitly. Thus address this non-linearity with predictor-corrector methods would just have the disadvantage of introducing additional robustness issues.
On the basis of the sequentially linear "saw-tooth" algorithm [7], cracking is solved implicitly, by removing broken beams one by one and computing equilibrium in between every removal [1]. The redistribution of forces is instantly taken into account avoiding time-discretization dependency of the cracking pattern.
Obviously, multiple beams exceed their breaking criterion at the same time, the beam to be removed at the current iteration is chosen as the one that exceeds its criterion the most:

$$\forall (i,j) \in \{(i,j) \mid P_{ij} > 1\} \qquad \min\left(\alpha_{ij} = \frac{1}{P_{ij}}\right) \tag{6}$$

As mentioned earlier, for the rest of the non-linearties, namely contact and frictional sliding, a predictor-corrector method is employed. The equilibrium is then solved with a method similar to Newton methods, in which the prediction of the centroids' displacements is made accounting for exact cohesive interactions, the elastic part of friction interactions, and a linearized approximation of contact interactions. Contact and friction interactions are only considered in the prediction if the contact between two particles has been detected at the previous iteration, similarly to the "open-close iteration" algorithm [8].
To compute the linear approximation of contact forces in function of centroids' displacements, we suppose that the two contacting particles are linked with a beam, analogously to cohesive interactions. The resulting contact force approximation is:

$$\delta F^{pred}_{cont,ij} = \frac{EL_{c,ij}}{l_{c,ij}} \left(\delta \underline{u}_i - \delta \underline{u}_j\right) . \underline{n} \tag{7}$$

Relaxation is also introduced to limit convergence issues, which are enhanced by the quasi-static framework and the disregard of damping effects. Relaxation is done, only considering a certain amount of the predicted displacement increment, if the residual increases or decreases too slowly:

$$\underline{u}^{k+1} = \underline{u}^{k} + h^{k+1}\delta\underline{u}^{k+1} \qquad h^{k+1} = \begin{cases} h^{k} & \text{if} \quad \delta\underline{r}^{k+1} \leq 1.e^{-4} \\ \dfrac{h^{k}}{2} & \text{if} \quad \delta\underline{r}^{k+1} > 1.e^{-4} \end{cases} \tag{8}$$

where $\underline{\delta u}^{k+1}$ is the predicted increment, $\underline{\delta r}^{k+1}$ is the residual increment and h^{k+1} is the relaxation factor at the current iteration $k+1$.

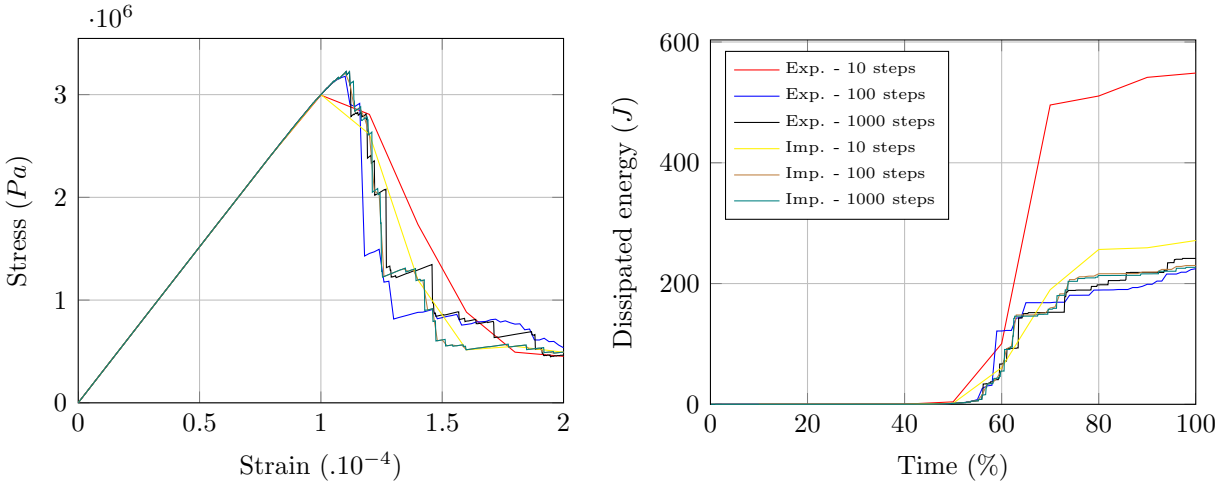
4 Results

Two simple loading cases are simulated to show the interest of implementing an implicit integration scheme for lattice discrete elements models, especially when accounting for cracking and contact. A comparison is made with an explicit integration of quasi-static equilibrium.

4.1 Tensile test

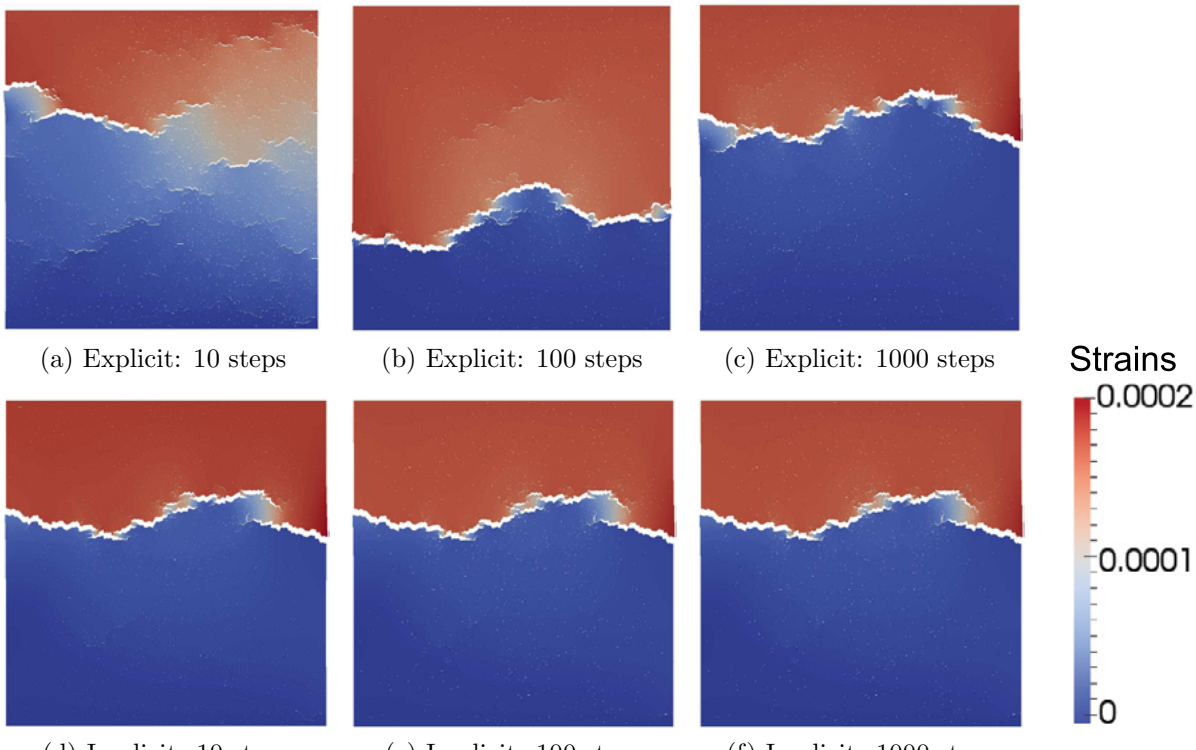
The first loading case is a direct tensile test. Fracture mechanisms are the main focus. Parameters are defined such as the tensile behavior is fragile, to the extent that after the peak load is reached, the tangent to the force-displacement curve is sometimes almost vertical. A total strain of 2.10^{-4} is imposed in 10, 100 or 1000 time-steps. Influence of the scheme, explicit or implicit, depending on the number of time-steps, on the cracking pattern and the fracture dissipated energy is studied.

As a result, cracking patterns (fig.3) are strongly dependent on the time-discretization with an explicit scheme, which locations vary as well as their localization level. In that case, the implicit scheme is efficient, cracking patterns are identical. From the dissipated energy point of view (fig.2), the interest of an implicit method is not necessarily obvious. The dissipated energy converges quickly as soon as the localization occurs. Indeed, from 10 to 100 time-steps the crack pattern passes from diffused to localized, important variation of the dissipated energy can be observed. However from 100 to 1000 time-steps, only the position of the localized crack changes, only small variations can be observed on the dissipated energy. An implicit scheme, serves here mostly to avoid important errors for coarse time-discretization, but the estimated energy for 10 time-steps remains slightly over-estimated.



(a) Stress-strain curves (b) Fracture dissipated energy

Figure 2: Influence of the integration scheme on the global response and dissipated energy during a tensile test



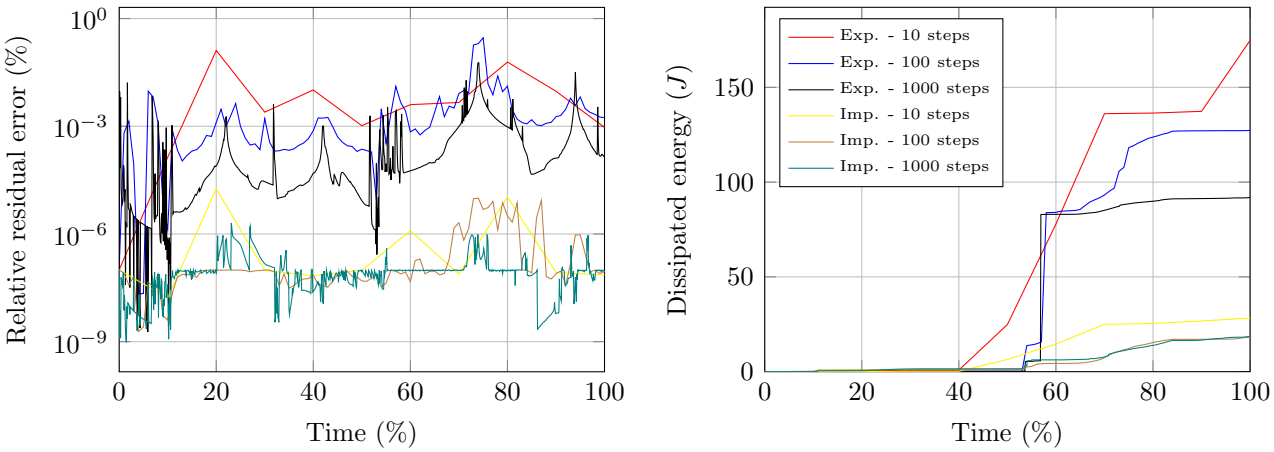
(a) Explicit: 10 steps (b) Explicit: 100 steps (c) Explicit: 1000 steps

(d) Implicit: 10 steps (e) Implicit: 100 steps (f) Implicit: 1000 steps

Figure 3: Influence of the integration scheme on the crack pattern under tensile loading

4.2 Cyclic test

This test is proceeded right after the previous tensile test. Starting with samples subject to a 2.10^{-4} tensile strain and with the same localized precracking (fig.3f), a compressive strain of -4.10^{-4} is applied. The purpose is to observe influence of the integration scheme on mechanisms occurring when the macroscopic crack is closed, namely contact and friction, which should occur logically around 50% of the load application. Every sample is precracked identically so as to only observe the influence of the integration scheme and the time-discretization. The load is applied in 10, 100 or 1000 time-steps.



(a) Relative residual error

(b) Friction dissipated energy

Figure 4: Influence of the integration scheme on the residual error and dissipated energy during the transition from uniaxial tension to compression

The figure (4a) shows the residual value at the end of every time-step. It illustrates the potential error of the computed solution, namely the difference between the computed internal forces and the imposed external forces. Regarding the implicit scheme, convergence is arbitrarily considered as reached when the residual error is lower than 1.10^{-7}. Convergence of the implicit scheme is mostly found at every time-step, which confirms the correct implementation of the algorithm. Additionally we can observe that residual error for the explicit scheme is often important, up to values reaching 50%. Such errors are considerably reducing the confidence in the parameters that could be identified with explicit integration schemes.

The figure (4b) shows the amount of dissipated energy by frictional sliding. As a direct consequence of the error observed previously with residuals, the computed values of dissipated energy with explicit integration schemes are overestimated. Inaccurate jump of the dissipated energy appears around 55% of the load application. This happens right after

the transition from tension to compression. The numerous detection of contact at that moment, and the important stiffness variation might explain the inaccuracy of the results, and the origin of the jump of dissipated energy. On the contrary, implicitly computed values are similar independently of the time-discretization, although the value computed in 10 time-steps is slightly overestimated, but convergence is observed for 100 and 1000 values.

5 Conclusion

In order to proceed to numerical testing, and more particularly to numerical identification of macroscopic models, requirements were a simple but representative model, with few physically meaningful parameters, and a robust, time-independent, and accurate solving algorithm. Unlike classic dynamic explicit solving procedures, the developed algorithm solves equilibrium implicitly in a quasi-static framework.
From the two short studies, for tensile and compression loadings, we can conclude that efforts invested to implement an implicit solving procedure were justified. Non-negligible improvement in terms of numerical identification of scalar values such as energies, independently of the time-discretization, have been observed. Besides choices relative to the implementation of the solving procedure, namely the choice of the predictor and the use of relaxation, are efficient from the convergence or the residual point of view.

Regarding goals of the model, strictly speaking, simplicity can hardly be disputed, however representativeness still can be argued. Further work is to be accomplished before a precise description of the overall behavior of quasi-brittle materials is possible with a single set of parameters. Among model's deficiencies, the still quite brittle failure under compression is the most concerning. Accounting for porosity's consequences seems to be one of the most encouraging trails. The introduction of porosity directly in the mesh or probabilistic distribution of Young's modulus, will be investigated.
Be that as it may, the choice of a description based mostly on statistical or geometrical details is promising, and as soon as the identification of the discrete model is set, numerical identification of macroscopic models will be undertaken.

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